HELMHOLTZ GEMEINSCHAFT

Open Science

JÜLICH FORSCHUNGSZENTRUM

Das Journal of Large-Scale Research Facilities oder: Wie Großgeräte eine DOI bekommen

Helmholtz Open Science Webinare zu Forschungsdaten
Webinar 26 – 27.04./07.05.15

Dr. Bernhard Mittermaier, Forschungszentrum Jülich, Zentralbibliothek
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Mission der Helmholtz-Gemeinschaft

„Wir erforschen Systeme hoher Komplexität unter Einsatz von Großgeräten und wissenschaftlichen Infrastrukturen gemeinsam mit nationalen und internationalen Partnern.“

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Das Großgerät wird im Abstract genannt …

„ First demonstrations of this setup at the coherence beamline of the PETRA III storage ring yield a highly divergent far-field diffraction pattern, from which the autocorrelation function of the near-field intensity distribution was obtained. “

DOI:10.1063/1.3698119

… oder im Acknowledgment

„And many thanks to the Alfred Wegener Institute for Polar and Marine Research (AWI) for providing the opportunity to join several research cruises across the Atlantic Ocean on RV Polarstern, especially the expeditions ANT-XXIII/10, ANT-XXIV/1, ANT-XXIV/4, ANT-XXV/5 and ANT-XXVI/1.“

doi:10.5194/amt-5-2391-2012

… oder irgendwo

In the finite element context of Alya, the proposed gluing method consists in adding new elements, referred to as extension elements. These elements are assembled *almost* like normal finite elements (during the Assembly task) and do not require any particular treatment. Therefore the gluing method inherits the parallel performance in Alya. Figure 4 shows the speedup obtained on a Blue-Gene Q.

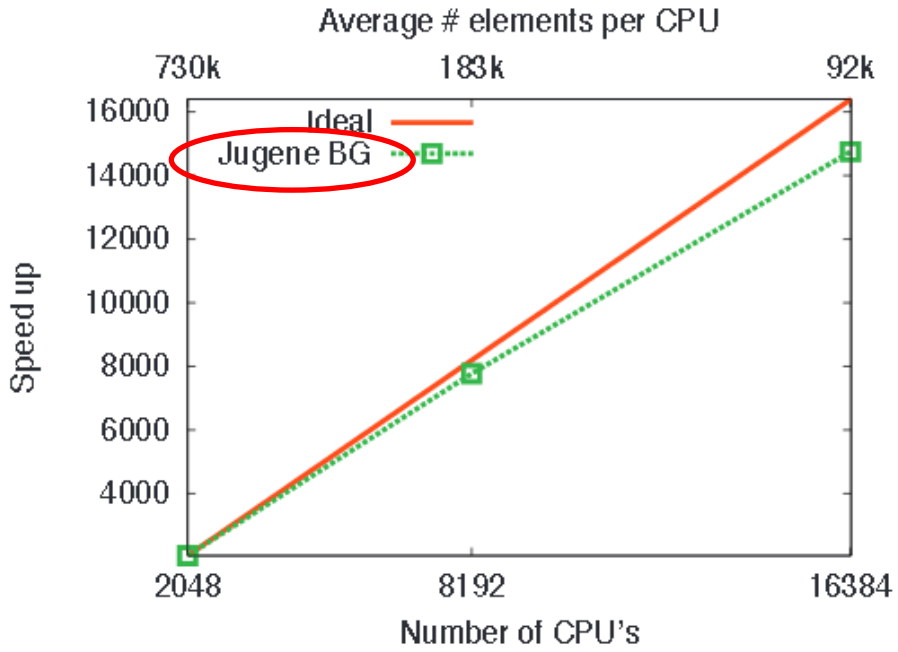


Figure 4 Alya speedup

DOI:10.1016/j.proeng.2013.08.013

… oder gar nicht.

Status quo

1. Die Nennung des Helmholtz-Zentrums / des Großgerätes erfolgt derzeit an unterschiedlichen Stellen in der Publikation (Einleitung, Methodenteil, Acknowledgement) oder sie fehlt ganz.
2. Sie erfolgt nicht auf normierte Weise, weshalb eine Gesamtauswertung (z.B. über eine Suche im Web of Science) praktisch kaum durchführbar ist.

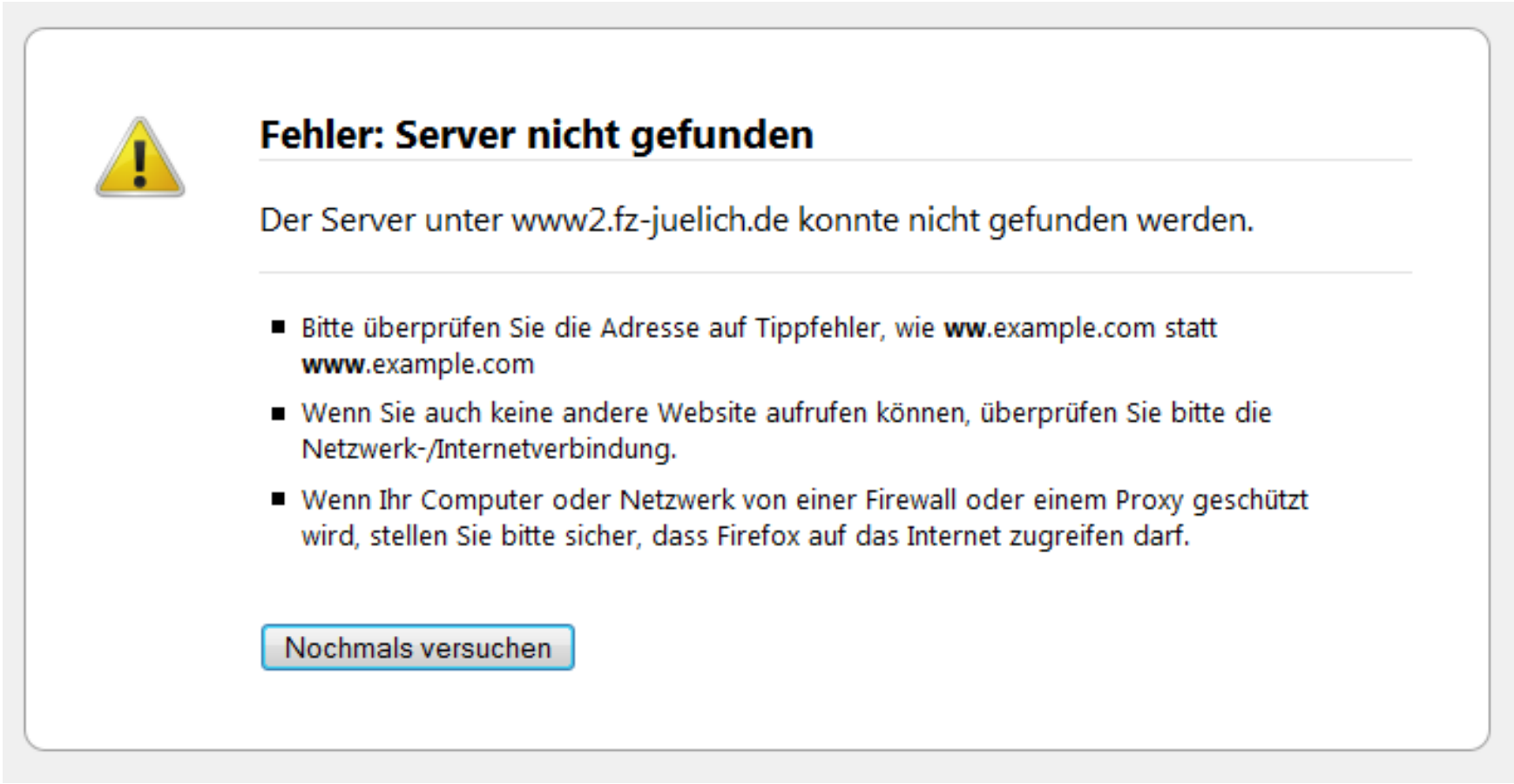
Die Erfolgsbilanz des Helmholtz-Gemeinschaft stellt sich in einer Kernkompetenz schlechter dar als sie ist.

Im Ansatz nicht schlecht

„This work was financially supported both by the PRACE First Implementation Project funded in part by the EUs 7th Framework Programme (FP7/2007–2013) under grant agreement no. RI-261557 and by Science Foundation Ireland (grant 08/HEC/I1450). Benchmarks were carried out on the Jugene [14] machine at Jülich, on Curie [13] at the CEA and on Fermi [15].“

[14] http://www2.fz-juelich.de/jsc/jugene

DOI:10.1016/j.cpc.2013.03.003


Fehler: Server nicht gefunden
Der Server unter www2.fz-juelich.de konnte nicht gefunden werden.
Bitte überprüfen Sie die Adresse auf Tippfehler, wie ww.example.com statt www.example.com
Wenn Sie auch keine andere Website aufrufen können, überprüfen Sie bitte die Netzwerk-/Internetverbindung.
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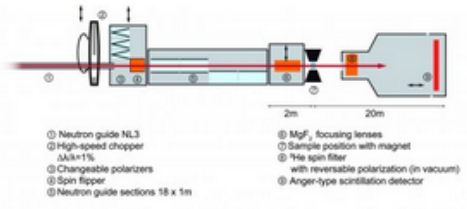
1. Für jedes Großgerät wird eine DOI vergeben („Digital Object identifier“; persistent). Die externen Nutzer sind gehalten (ggf. in einer Benutzungsordnung, in einer Messzeitbewilligung etc.), diese DOI zu zitieren. Dadurch erfolgt die Referenzierung auf das Großgerät stets an der gleichen Stelle (in den Referenzen der Publikation) und in der gleichen Form (über die DOI), was eine Gesamtauswertung möglich macht.
2. Eine DOI muss zu einem Objekt im Internet auflösen. Dieses Objekt ist eine kurze Beschreibung des Großgerätes sein, vgl. z.B. die Instrumentenbeschreibung am MLZ.

KWS-1

Small angle scattering diffractometer



The KWS-1 is dedicated to high resolution measurements due to its 10 % wavelength selector. This property is interesting for highly ordered or highly monodisperse samples. With the foreseen chopper the wavelength uncertainty can be reduced further to ca. 1 %. The scientific background of KWS-1 is placed in magnetic thin films. Magnetic samples will be studied with the full polarization analysis including incident beam polarization and polarization analysis of the scattered neutrons. In front of the collimation, a 3-cavity polarizer with V-shaped mirrors is placed. The full bandwidth of 4.5 to 20 Å will be covered with min. 90 % (95 % typical) polarization. A radio frequency spin flipper allows for changing the polarization. The polarization analysis will be realized with 3He-cells which will be optimized for the used wavelength and scattering angle. Vertical magnets will be provided to render the magnetic field at the sample position. Thin films can be well studied in the grazing incidence geometry – the method is called grazing incidence small angle neutron scattering (GISANS). A newly installed hexapod will allow for positioning the sample with 0.01 mm and 0.01° precision.

Classical soft-matter systems will be investigated on KWS-1 if the resolution is needed. Biological samples can be handled due to the detector distance of ca. 1 m, which will allow for maximal scattering angles of Q = 0.5 $Å^{-1}$.

The MgF_2 lenses are used for the high flux mode with large sample areas, while the resolution stays in the classical SANS range. These enhanced intensities allow for real time measurements in the 1/10 second region (typical 1 s).

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Operated by

Jülich Centre for Neutron Science

Gallery

Lösung

3. Mit Blick auf die Akzeptanz durch die Nutzer und mit Blick auf eine größtmögliche Verbreitung wurde die **Open Access-Zeitschrift „Journal of large-scale research facilities“ (JLSRF)** gegründet, die derartige Dokumente enthält. Die Zentralbibliothek des Forschungszentrums Jülich übernimmt die organisatorische Abwicklung. 

4. Die Beschreibungen werden durch Personen erstellt, die für das jeweilige Großgerät verantwortlich sind. Sie werden als anonyme Werke publiziert, um keine persönlichen Zitierungen zu „erzwingen“:
   Heinz Maier-Leibnitz Zentrum. (2015). BioDiff - Version 1. *Journal of large-scale research facilities*,1, A7. http://dx.doi.org/10.9999/example-doi.

3. Statt Peer Review findet lediglich ein Editorial Review statt mit Editoren aus den einzelnen Helmholtz-Zentren.

Vorlage

Journal of **large-scale research** facilities

Journal of large-scale research facilities, 1, A1 (2015)

http://dx.doi.org/10.9999/example-doi

eine DOI für ein Messgerät

Published: 01.01.2015

Abbreviation and full name of the large-scale research facility as title - Version 1

Versionierung/Historie

Instrument Affiliation

Instrument Scientists:
- J. Doe, Affiliation, Contact Information
- R. Who, Affiliation, Contact Information

Zitieren

Heinz Maier-Leibnitz Zentrum. (2015a). Instrument. *Journal of large-scale research facilities*, *1*, A2. http://dx.doi.org/10.9999/example-doi

Heinz Maier-Leibnitz Zentrum. (2015b). Instrument - Version 1. *Journal of large-scale research facilities*, *1*, A5. http://dx.doi.org/10.9999/example-doi

Instrument Affiliation. (2015). Instrument - Version 3. *Journal of large-scale research facilities*, *1*, A10. http://dx.doi.org/10.9999/example-doi

Beispiel

Journal of large-scale research facilities

Journal of large-scale research facilities, 1, A1 (2015) http://dx.doi.org/10.9999/example-doi

Published: 01.01.2015

BioDiff: The New Diffractometer for Crystals with Large Unit Cells - Version 1

Heinz Maier-Leibnitz Zentrum

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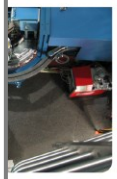
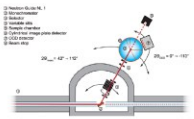
Abstract: The BioDiff diffractometer is a new instrument built at the Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II) in collaboration between the Forschungszentrum Jülich and the FRM II. It is optimised for studies of crystals with large unit cells and its main application lies in the structural analysis of protein crystals, more precisely in the determination of the position of the hydrogen atoms that are easily seen by neutron scattering but are normally not observed by X-ray crystallography. The BioDiff instrument is now in full user operation.

1 Instrument description

Since the human genome has been decoded and sequencing of the genome of other organisms has become a standard procedure the resulting information on the proteins encoded in these genomes can be used to express them in bacterial or yeast based expression systems and thereby study their interplay and function. One of the overall goals is a better understanding of the metabolism of a cell and thereby improving drugs and suppress side effects since they are tailored to attack only the part of the cell metabolism they are supposed to do so. In order to understand the function of a protein the knowledge of its three dimensional structure is a prerequisite. Often intermediate steps in the course of the catalytic process of a protein can be trapped and investigated with structure analysing techniques exhibiting atomic resolution, e.g. with X-ray or neutron diffraction. Here, the instrument BioDiff is able to perform neutron diffraction studies on protein crystals with comparatively large unit cells. The unique feature of BioDiff as compared to comparable instruments (e.g., LADI-III at ILL) is that the incident neutron wavelength can be adapted to the unit cell size of the sample crystal. Figure 1 shows a schematic view of the BioDiff instrument from the top and a corresponding picture when the biological shielding has been partly removed.
By Bragg reflection from a pyrolytic graphite crystal (002-reflection) neutrons are selected from the white spectrum of the neutron guide NL1 and pass through a first boron carbide adjustable slit and



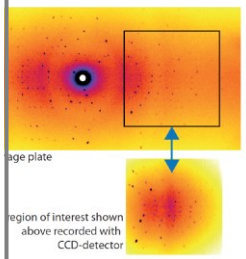


the BioDiff instrument (top) and a picture taken from a similar viewpoint removed (left).

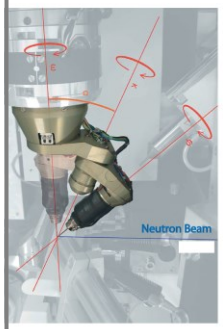
acts as $\lambda/2$ filter. Together with the pyrolytic graphite crystal it forms λ/λ of $\sim 2.5\%$. Before entering the cylindrical drum of the image plate by variable slits to fit to the sample size.
o detectors. The cylindrical image plate detector ($400\,mm$ in diameter and ng roughly half of the total 4π solid angle. It can be read out with three μm, $250\,\mu m$ and $500\,\mu m$. As an alternative, one can lower the image plate tron sensitive scintillator which is imaged onto a CCDchip.
rves as second detector but can also be used for the fast alignment of the o the neutron beam. The size of the scintillator is $197\,mm \times 197\,mm$ and its $100\,mm$. It can be moved around the sample to achieve 2Θ-values between can be displaced vertically by $100\,mm$. Measuring at several positions, the hievable with the CCD-detector amounts also to 2π.
letector types showed that the CCD-camera detector is comparable in sen- tector, but covers only a smaller area (compare Figure 2). However, taking dout times of the image plate detector, the CCD-detector is an alternative g crystals. Here, the faster readout of the CCD-chip pays off even if the ler area.
of user operation 14 complete data sets of protein and DNA crystals were Diff.

nt development and upgrades

as to be taken off the instrument when one wants to tilt it in order to in- e data set. This increases the risk to damage the crystal either mechanically king under cryo-conditions. With a mini-kappa goniometer head as shown ded and an optimised tilt geometry can be chosen using special strategy ollect the data more efficiently.
tream can in some cases improve the crystal quality due to hydration and D2O vapour (already tested at Proteros in Martinsried). It will also enable s in low resolution crystallographic applications: e.g. lipids or detergents m the protein in membrane protein crystals. Better Lithium-ceramic flight background from air scattering of the primary beam. Illumination of the cal fibre will allow to prepare and maintain intermediate states of photo-



nage plate detector (upper part) compared to the same settings for



variable tilt of the crystal while keeping it in the cold nitrogen gas aken from Brockhauser, S. and Ravelli, R. B. G. and McCarthy, A. A.

extend the existing wavelength range down to about $1.8\,\AA$ utilising an monochromator. This will close the gap to the thermal single crystal ding the application range of BioDiff to medium compound crystals.

peration where the protein crystal is typically mounted in a sealed ne mother liquor BioDiff offers a standard Oxford Cryosystems 700+ nts in a nitrogen gas stream down to $90\,K$. Additionally, a closed cycle s temperatures down to $4\,K$ in vacuum for small compound crystals.

s

he neutron structure analysis of proteins, especially the determination ical fields of interest are:
otonation states of amino acids in the active center)
tion shell of proteins
by hydrogen bonds
a monitor of structural stability/flexibility
proven to produce good quality crystallographic data sets and is now

G. and McCarthy, A. A. (2013). The use of a mini-k goniometer head in hy diraction experiments. *Acta Crystallographica Section D: Biological* -1251. http://dx.doi.org/10.1107/S0907444913003880